Chemistry42: An AI-Driven Platform for Molecular Design and Optimization

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Abstract

Chemistry42 is a software platform for de novo small molecule design and optimization that integrates Artificial Intelligence (AI) techniques with computational and medicinal chemistry methodologies. Chemistry42 efficiently generates novel molecular structures with optimized properties validated in both in vitro and in vivo studies and is available through licensing or collaboration. Chemistry42 is the core component of Insilico Medicine’s Pharma.ai drug discovery suite. Pharma.ai also includes PandaOmics for target discovery and multiomics data analysis, and inClinico—a data-driven multimodal forecast of a clinical trial’s probability of success (PoS). In this paper, we demonstrate how the platform can be used to efficiently find novel molecular structures against DDR1 and CDK20.